

1(2H)-Naphthalenone, octahydro-, trans-

Other names:	trans-«alpha»-Decalone trans-1-Decalone trans-Bicyclo[4.4.0]decan-2-one Octahydro-2H-naphthalen-1-one, trans- trans-Decalone-1 1-Decalone, trans- Octahydro-1(2H)-naphthalenone, (E)- trans-bicyclo(4.4.0)decan-1-one
Inchi:	InChI=1S/C10H16O/c11-10-7-3-5-8-4-1-2-6-9(8)10/h8-9H,1-7H2/t8-,9+/m1/s1
InchiKey:	AFEFRXAPJRCTOW-BDAKNGLRSA-N
Formula:	C10H16O
SMILES:	O=C1CCCC2CCCCC12
Mol. weight [g/mol]:	152.23
CAS:	21370-71-8

Physical Properties

Property code	Value	Unit	Source
gf	-16.17	kJ/mol	Joback Method
hf	-266.47	kJ/mol	Joback Method
hfus	9.04	kJ/mol	Joback Method
hvap	42.62	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.546		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
tb	526.58	K	Joback Method
tc	766.02	K	Joback Method
tf	292.48	K	Joback Method
vc	0.484	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.13	J/mol×K	526.58	Joback Method

cpg	346.46	J/mol×K	566.49	Joback Method
cpg	366.51	J/mol×K	606.39	Joback Method
cpg	385.29	J/mol×K	646.30	Joback Method
cpg	402.83	J/mol×K	686.21	Joback Method
cpg	419.17	J/mol×K	726.11	Joback Method
cpg	434.33	J/mol×K	766.02	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	346.20	K	0.10	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21370718&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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